Reply to comment on "On the continuum-scale modeling of gravity-driven fingers in unsaturated porous media: The inadequacy of the Richards equation with standard monotonic constitutive relations and hysteretic equations of state" by Mehdi Eliassi and Robert J. Glass

M. Eliassi and R. J. Glass

Flow Visualization and Processes Laboratory, Sandia National Laboratories, Albuquerque, New Mexico, USA

Received 30 November 2002; accepted 9 April 2003; published 18 September 2003.

INDEX TERMS: 1829 Hydrology: Groundwater hydrology; 1866 Hydrology: Soil moisture; 1875 Hydrology: Unsaturated zone; *KEYWORDS:* capillary hysteresis, extended Darcy flux relations, gravity-driven fingers, Richards equation, truncation error–induced numerical oscillations, wetting front instabilities

Citation: Eliassi, M., and R. J. Glass, Reply to comment on ''On the continuum-scale modeling of gravity-driven fingers in unsaturated porous media: The inadequacy of the Richards equation with standard monotonic constitutive relations and hysteretic equations of state'' by Mehdi Eliassi and Robert J. Glass, *Water Resour. Res.*, *39*(9), 1264, doi:10.1029/2003WR002053, 2003.

1. Introduction

[1] In the mid-1980s the discovery of finger persistence, both for constant infiltration as well as in subsequent infiltration events [*Glass et al.*, 1988], suggested that standard unsaturated flow theory applied to gravity-driven fingering (GDF) was incomplete. Subsequent discovery of the nonmonotonic behavior in saturation (and thus pressure) at the finger tip [*Glass et al.*, 1989] clenched this fate for the traditional conceptualization. While a standard hysteretic mechanism can fully explain finger persistence following from the nonmonotonic behavior at the tip, the cause (i.e., the initiation) of nonmonotonicity within the finger could not be explained by standard theory. This critical point lied dormant for many years. In the meantime, many assumed that standard porous-continuum theory, in combination with hysteretic equations of state, contained all the relevant physics and was sufficient to explain GDF. Therefore when *Nieber* [1996] presented his results, they were embraced as "the first to model experimentally observed unstable fingered flow successfully" [*Deinert et al.*, this issue, second paragraph] (hereinafter referred to as DPCSS). *Nieber*'s [1996] simulations were purported to be solutions of the traditional unsaturated flow governing equation, the Richards equation (RE). However, we demonstrated that such assumed physics; that is, the RE in combination with standard monotonic properties (SMP) (defined by standard constitutive relations and hysteretic equations of state [*Mualem*, 1976; *van Genuchten*, 1980]) was not sufficient to model GDF [*Eliassi and Glass*, 2001a].

[2] We are happy to see that our work has caused others to recognize the insufficiency of traditional theory. Of course, recognizing that traditional theory (i.e., the RE) cannot fully represent GDF requires the recognition that *Nieber*'s [1996] solution of the RE can only "mimic" GDF (DPCSS, first paragraph). We note, however, that such recognition cannot be found in six other works [*Ritsema et al.*, 1998a, 1998b; *Nguyen et al.*, 1999a, 1999b; *Nieber et al.*, 2000; *Ritsema and Dekker*, 2000] that faithfully used the basic numerical method suggested by *Nieber* [1996] after it was developed. In fact, within all this work a statement is made that the governing equation being solved is the RE and that *van Genuchten* [1980] equations are used to describe (water) saturation-capillary pressure and saturation-hydraulic conductivity relations. Critical to the mimic is the use of downwind averaging of the hydraulic conductivity in the numerical solution approach. However, as we showed [*Eliassi and Glass*, 2001a], the downwind averaging does more than simply ''adjust the permeability'' at the wetting front as was suggested by DPCSS (first paragraph). Actually, downwind averaging induces a numerical error that can be large enough to modify the underlying governing equation such that RE is no longer being solved. Of course, with grid refinement this numerical error reduces and the GDF response vanishes. DPCSS states that we have ''exaggerated'' (final paragraph) our critique of *Nieber* [1996]. Of course, we do not believe that we have exaggerated our critique. In light of this comment we endeavor to explain, once again, our results and their significance in section 2 below.

[3] More recently, we have gone beyond the RE to consider its extension to include the experimentally observed hold-back-pile-up (HBPU) effect [*Eliassi and Glass*, 2001b, 2002] critical for the porous-continuum modeling of GDF. By postulating the HBPU effect as physically tied to wetting front sharpness, the HBPU can be mathematically formulated in a variety of ways to include hypodiffusive, hyperbolic, and mixed spatial-temporal forms. For each an extended flux relation comprised of the Darcy-Buckingham flux plus an additional component due to the HBPU effect can be inferred. While parallels for each extended flux relation can also be found in the multiphase literature, it remains to be seen whether such porous-continuum-scale models can be applied such as to increase our basic understanding of the GDF process. DPCSS have suggested that the recent work of

Deinert et al. [2002] and *Dautov et al.* [2002] shed light on extended theory in the context of modeling GDF. While such discussion may prove premature, we address extended theory and these preliminary works in section 3 below.

[4] Finally, we agree with DPCSS that an increased understanding of GDF must come from a consideration of pore-scale physics. In fact, one of us (Glass) has been involved for quite some time in both experiments, where pore-scale behavior can be observed [e.g., *Mortensen et al.*, 2001; *Glass et al.*, 2000; *Zhong et al.*, 2001] as well as the development of alternative pore-scale modeling approaches for two-phase immiscible displacements in porous media and fractures. Indeed, to our knowledge, the first simulations of GDF were not accomplished by *Nieber* [1996] (DPCSS, first paragraph) but by *Glass and Yarrington* [1989], where a pore-scale approach, based on Modifications of Invasion Percolation (MIP), was used. A full discussion of this work as it pertains to the GDF is far beyond the scope of this reply. Instead, we refer the reader to *Glass and Yarrington* [1996], *Glass et al.* [2001], and, most recently, *Glass and Yarrington* [2003] as well as to the large number of references contained therein.

2. Nieber and Colleagues Were Not Solving RE

[5] In previous work [*Eliassi and Glass*, 2001a] we formally evaluated the leading truncation error (LTE) due to discretization to yield an equation comprised of the original RE along with other additional terms arising from LTE. This equation, often referred to as the "modified governing equation," is the actual partial differential equation being solved during the numerical solution steps [e.g., see *Warming and Hyett*, 1974]. On the basis of our results, where downwind averaging yields a finger response, the total LTE is mainly dominated by the LTE for the gravity term in the RE. Thus, considering only the gravity term's LTE, the modified governing equation for constant grid spacing is given by

$$\Gamma\frac{\partial\Psi}{\partial\tau}-\left[\frac{\partial}{\partial\eta}\left(\kappa\frac{\partial\Psi}{\partial\eta}\right)+\frac{\partial}{\partial\xi}\left(\kappa\frac{\partial\Psi}{\partial\xi}\right)\right]-\frac{\partial\kappa}{\partial\xi}=\left(w\frac{\Delta\xi}{2}\right)\frac{\partial^2\kappa}{\partial\xi^2}, \tag{1}$$

where the left-hand side represents a dimensionless form of the RE in two dimensions and the right-hand side (RHS) is the gravity term's LTE arising from the downwind averaging; $w < 0$ is the weighting factor suggested by *Nieber* [1996], and $\Delta\xi$ is the dimensionless grid spacing in the direction of gravity (refer to *Eliassi and Glass* [2001a] for additional explanation). We demonstrated [*Eliassi and Glass*, 2001a] that it is the presence of the LTE term on the RHS of equation (1) that allows *Nieber*'s [1996] approach to mimic GDF. Of course, with grid refinement (i.e., as $\Delta\xi \to 0$) the RHS of equation (1) becomes small enough for the GDF response to disappear.

[6] Thus in the averaging method used by Nieber, GDF arises through a numerical artifact that is fit with a numerical grid-based parameter, $w\Delta\xi/2$. We note, however, that the mimic of GDF provided by this approach is quite good, especially when $\Delta\xi$ and w are calibrated against data. One also finds that the artificial LTE-induced fingers have the same qualitative behavior as physical fingers with respect to material nonlinearity (i.e., n parameter in *van Genuchten*'s [1980] model) and/or to initial moisture content.

[7] In any case, as we stated in the conclusion of our previous work [*Eliassi and Glass*, 2001a, section 5], the use of Nieber's approach to study GDF is problematic. An approach that is ultimately a "curve fit" cannot yield new understanding within the range of its data set, and outside of its data range the curve fit is simply extrapolation and must be validated before it can be used.

[8] Interpretation of extrapolated results can often yield misunderstanding instead of increased understanding. In this sense we lament that one must exercise caution regarding the use of interpretations based on numerical results within all papers that have employed Nieber's method [e.g., *Nieber*, 1996; *Ritsema et al.*, 1998a, 1998b; *Nguyen et al.*, 1999a, 1999b; *Nieber et al.*, 2000; *Ritsema and Dekker*, 2000].

3. On Extended Physics and Relevance of the Recent Work by DPCSS and Colleagues

[9] Our conclusion, as stated in our previous work, was [*Eliassi and Glass*, 2001a, p. 2019]

> Thus the RE along with standard monotonic hydraulic properties does not contain the critical physics required to model gravity-driven fingers and must be considered inadequate for unsaturated flow in initially dry, highly nonlinear, and hysteretic media where these fingers occur.

Possible alternatives to the standard approach were listed to [*Eliassi and Glass*, 2001a, p. 2032]

> . . .include but are not limited to a dynamic capillary pressure resulting in nonstandard equations of state; modified nonmonotonic constitutive relations for the relative permeability; and/or entirely different formulations of the flux law itself.

We have gone on to consider additional physics and invite DPCSS and others to consider our recent work [*Eliassi and Glass*, 2002], where we identify the experimentally observed HBPU effect and mathematically model the HBPU in a variety of forms. Support for each of these forms can be found within extended theory for single-phase and multiphase flow and, interestingly, from very different underlying conceptualizations of the possible physics. The form of interest with regard to the comment of DPCSS is the third-order, mixed spatial-temporal form with an underlying conceptualization based on the theory of dynamic capillary pressure such as that of *Hassanizadeh and Gray* [1993].

[10] DPCSS suggest that the work of *Deinert et al.* [2002] provides "further insight" (paragraph 3) into the GDF problem, in particular, through the interpretation of experimental data with the concept of "dynamic pressure." *Deinert et al.* [2002] used the measured saturation profile along a finger, the measured hydraulic conductivity as a function of moisture content, and the standard Darcy's law to back-calculate the pressure gradient along the profile. This gradient was then used to project a nonabsolute pressure as a function of moisture content. As a prelude, we note that the application of Darcy's law to yield finger behavior was first suggested over a decade ago [*Glass et al.*, 1989]. There the analysis was restricted to the saturated finger tip region and allowed derivation of a relationship for

finger tip length, L_s, as a function of water entry pressure at the finger tip, ψ_{we}, air entry pressure behind the tip where the tip begins to desaturate, ψ_{ae}, hydraulic conductivity of the tip region, K_f, and flux through the finger, q_f. This relation was written simply as [see *Glass et al.*, 1989, equation (4)]

$$L_s = \frac{\psi_{\omega\varepsilon} - \psi_{\alpha\varepsilon}}{1 - \frac{q_f}{K_f}}. \quad (2)$$

We note in passing that a ‘‘dynamic’’ water entry pressure function could be obtained directly from equation (2) by the measurement of finger tip length for experimental fingers with a variety of fluxes. Regardless, while equation (2) was written for constant saturation zones where it applies with few assumptions, DPCSS have assumed constant flux along the core of a finger and generalized this relation to apply outside the constant saturation region of the profile. Application of their equation (1) to the data of *Deinert et al.* [2002] yields the pressure-saturation history shown in their Figure 1. We must note, however, that this general behavior has been recognized previously [e.g., *Glass et al.*, 1989; *Selker et al.*, 1992; *Liu et al.*, 1994a, 1994b]. We are happy that the authors now understand this behavior as a direct consequence of physics that is not part of the standard RE + SMP.

[11] DPCSS also suggest a relation between the results in their Figure 1 and the recent work of *Dautov et al.* [2002], who consider a dynamic capillary pressure concept to model GDF. The approach used by *Dautov et al.* [2002] essentially involves numerical solution of the RE coupled with a first-order initial value problem representing a dynamic capillary pressure. Although in the original formulation of *Hassanizadeh and Gray* [1993] dynamic capillary pressure equation includes a temporal derivative of saturation, *Dautov et al.* [2002] have rewritten this equation in terms of the temporal derivative of dynamic pressure. Their numerical simulation illustrates a nonmonotonic response such as seen in GDF and suggests that a third-order, mixed-form flux law based on a dynamic capillary pressure, such as we present in our recent work [*Eliassi and Glass*, 2002], can indeed yield an appropriate HBPU as required for a porous-continuum approach to model GDF. We note that in our recent work [*Eliassi and Glass*, 2002, section 4.3] we were skeptical that a mixed-form flux derived directly from the theory of *Hassanizadeh and Gray* [1993] could yield the proper HBPU effect at the wetting front. Regardless, assuming the results of *Dautov et al.* [2002] to be correct, we wonder at DPCSS's statements that their back-calculated ‘‘dynamic pressure’’ shown in their Figure 1 ‘‘leads to instability when used in conjunction with a continuum approach’’ (paragraph 4). Once again, we emphasize that the presentation in their Figure 1 is simply a system response and thus is a direct consequence of physics beyond the standard RE + SMP rather than a cause.

4. Conclusion

[12] The RE has been used with great success in a wide variety of situations in hydrology. However, the RE in conjunction with SMP does not work where GDF forms. Paraphrasing the words of *Feynman* [1992], if the model does not fit nature, it is wrong. We must then develop a new and more comprehensive theory that can properly model GDF for the range of parameter space where it occurs. We are very happy that our work [*Eliassi and Glass*, 2001a] has instigated research along these lines by others, and we encourage a reading of our own such work [*Eliassi and Glass*, 2002]. It is indeed unknown whether such extended physics can be appropriately incorporated into a continuum approach to fully model GDF. However, as can be seen in the recent pore-scale simulations using MIP [*Glass and Yarrington*, 2003], GDF and its nonmonotonic signature can indeed be modeled with an appropriate, physically based mechanistic model.

References

Dautov, R. Z., A. G. Egorov, J. L. Nieber, and A. Y. Sheshukov, Simulation of two-dimensional gravity-driven unstable flow, in *Proceedings of XIV International Conference on Computational Methods in Water Resources*, edited by S. M. Hassanizadeh et al., pp. 9–16, Delft Univ. of Tech., Delft, Netherlands, 2002.

Deinert, M., J.-Y. Parlange, T. S. Steenhuis, K. Ünlü, J. S. Selker, and K. B. Cady, Real-time measurement of water profiles in a sand using neutron radiography, in *Proceedings of the Twenty-Second Annual AGU Hydrology Days*, edited by J. A. Ramirez, pp. 56–61, AGU, Washington, D. C., 2002.

Deinert, M., J.-Y. Parlange, K. B. Cady, T. S. Steenhuis, and J. S. Selker, Comment on ‘‘On the continuum-scale modeling of gravity-driven fingers in unsaturated porous media: The inadequacy of the Richards equation with standard monotonic constitutive relations and hysteretic equations of state’’ by Mehdi Eliassi and Robert J. Glass, *Water Resour. Res.*, *39*, doi:10.1029/2002WR001785, in press, 2003.

Eliassi, M., and R. J. Glass, On the continuum-scale modeling of gravity-driven fingers in unsaturated porous media: The inadequacy of the Richards equation with standard monotonic constitutive relations and hysteretic equations of state, *Water Resour. Res.*, *37*, 2019–2035, 2001a.

Eliassi, M., and R. J. Glass, Porous continuum-scale modeling of gravity-driven fingers in unsaturated porous materials: Extended flux laws and numerical simulations, *Eos Trans. AGU*, *82*(47), Fall Meet. Suppl., Abstract H52A-0377, 2001b.

Eliassi, M., and R. J. Glass, On the porous-continuum modeling of gravity-driven fingers in unsaturated materials: Extension of standard theory with a hold-back-pile-up effect, *Water Resour. Res.*, *38*(11), 1234, doi:10.1029/2001WR001131, 2002.

Feynman, R., *The Character of Physical Law*, Penguin, London, 1992.

Glass, R. J., and L. Yarrington, Analysis of wetting front instability using modified invasion percolation theory, *EOS Trans. AGU*, *70*(43), Fall. Meet. Suppl., 1117, 1989.

Glass, R. J., and L. Yarrington, Simulation of gravity-driven fingering in porous media using a modified invasion percolation model, *Geoderma*, *70*, 231–252, 1996.

Glass, R. J., and L. Yarrington, Mechanistic modeling of fingering, non-monotonicity, fragmentation, and pulsation within gravity/buoyant destabilized two-phase/unsaturated flow, *Water Resour. Res.*, *39*(3), 1058, doi:10.1029/2002WR001542, 2003.

Glass, R. J., T. S. Steenhuis, and J.-Y. Parlange, Wetting front instability as a rapid and far-reaching hydrologic process in the vadose zone, *J. Contam. Hydrol.*, *3*, 207–226, 1988.

Glass, R. J., T. S. Steenhuis, and J.-Y. Parlange, Mechanism for finger persistence in homogenous unsaturated, porous media: Theory and verification, *Soil Sci.*, *148*, 60–70, 1989.

Glass, R. J., S. H. Conrad, and W. Peplinski, Gravity-destabilized nonwetting phase invasion in macroheterogeneous porous media: Experimental observations of invasion dynamics and scale analysis, *Water. Resour. Res.*, *36*, 3121–3137, 2000.

Glass, R. J., S. H. Conrad, and L. Yarrington, Gravity destabilized nonwetting phase invasion in macroheterogeneous porous media: Near-pore-scale macro modified invasion percolation simulation of experiments, *Water. Resour. Res.*, *37*, 1197–1207, 2001.

Hassanizadeh, S. M., and W. G. Gray, Thermodynamic basis of capillary pressure in porous media, *Water Resour. Res.*, *29*, 3389–3406, 1993.

Liu, Y., T. S. Steenhuis, J. S. Selker, and J.-Y. Parlange, Formation and persistence of fingered flow in coarse grained soils under different moisture contents, *J. Hydrol.*, *159*, 187–195, 1994a.

Liu, Y., T. S. Steenhuis, J. S. Selker, and J.-Y. Parlange, Closed-form solution for finger width in sandy soils at different water contents, *Water Resour. Res.*, *30*, 949–952, 1994b.

Mortensen, A. P., R. J. Glass, K. Hollenbeck, and K. H. Jensen, Visualization of microscale phase displacement processes in retention and outflow experiments: Nonuniqueness of unsaturated flow properties, *Water Resour. Res.*, *37*, 1627–1640, 2001.

Mualem, Y., A new model for predicting the hydraulic conductivity of unsaturated porous media, *Water Resour. Res.*, *12*, 513–522, 1976.

Nguyen, H. V., J. L. Nieber, C. J. Ritsema, L. W. Dekker, and T. S. Steenhuis, Modeling gravity driven unstable flow in a water repellent soil, *J. Hydrol.*, *215*, 202–214, 1999a.

Nguyen, H. V., J. L. Nieber, P. Oduro, C. J. Ritsema, L. W. Dekker, and T. S. Steenhuis, Modeling solute transport in a water repellent soil, *J. Hydrol.*, *215*, 188–201, 1999b.

Nieber, J. L., Modeling finger development and persistence in initially dry porous media, *Geoderma*, *70*, 207–229, 1996.

Nieber, J. L., T. W. J. Bauters, T. S. Steenhuis, and J.-Y. Parlange, Numerical simulation of experimental gravity-driven unstable flow in water repellent sand, *J. Hydrol.*, *231–232*, 295–307, 2000.

Ritsema, C. J., and L. W. Dekker, Preferential flow in water repellent sandy soils: Principles and modeling implications, *J. Hydrol.*, *231–232*, 308–319, 2000.

Ritsema, C. J., L. W. Dekker, J. L. Nieber, and T. S. Steenhuis, Modeling and field evidence of finger formation and finger recurrence in a water repellent sandy soil, *Water Resour. Res.*, *34*, 555–567, 1998a.

Ritsema, C. J., J. L. Nieber, L. W. Dekker, and T. S. Steenhuis, Stable or unstable wetting fronts in water repellent soils—Effect of antecedent soil moisture content, *Soil Tillage Res.*, *47*, 111–123, 1998b.

Selker, J. S., P. Leclerq, J.-Y. Parlange, and T. S. Steenhuis, Fingered flow in two dimensions: 1. Measurements of matric potential, *Water Resour. Res.*, *28*, 2513–2521, 1992.

van Genuchten, M. T., A closed-form equation for predicting the hydraulic properties of unsaturated soils, *Soil Sci. Soc. Am. J.*, *44*, 892–898, 1980.

Warming, R. F., and B. J. Hyett, The modified equation approach to the stability and accuracy analysis of finite-difference methods, *J. Comput. Phys.*, *14*, 159–179, 1974.

Zhong, L., A. Mayer, and R. J. Glass, Visualization of surfactant-enhanced nonaqueous phase liquid mobilization and solubilization in a two-dimensional micromodel, *Water Resour. Res.*, *37*, 523–537, 2001.

M. Eliassi and R. J. Glass, Flow Visualization and Processes Laboratory, Sandia National Laboratories, Albuquerque, NM 87158-0735, USA. (meliass@sandia.gov; rjglass@sandia.gov)